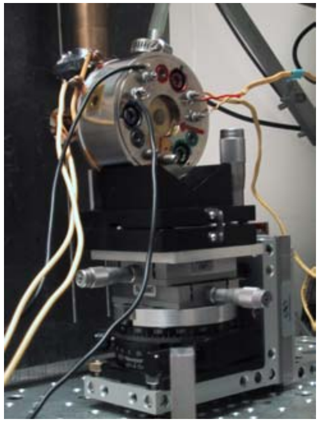
High Pressure Behavior of Negative Thermal Expansion Materials

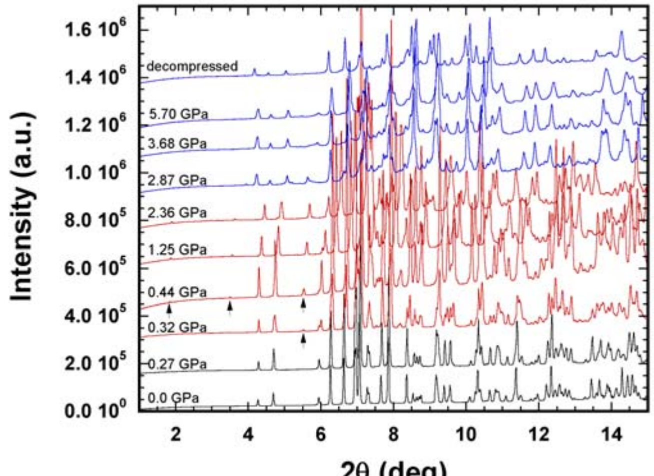
Angus P. Wilkinson, Georgia Institute of Technology, DMR-0203342

The thermal expansion characteristics of a material, that is how its dimensions change with temperature, are crucial to the construction of reliable devices that are subject to temperature changes.

Most materials expand on heating, but there are some substances that display negative thermal expansion (NTE), that is they shrink on heating. This can be exploited by preparing parts that contain a mixture of a normal material and one that shrinks on heating (to make a composite), and hence tuning the parts overall thermal expansion. During the preparation of composites high pressure is sometimes needed and this can result in the unwanted transformation of the NTE material to another crystalline phase that does not show NTE or to a glass (amorphous material). We are studying this behavior to better understand how, when and why it happens.



(left) Diamond anvil cell (DAC) recently loaded with liquid nitrogen pressure transmitting medium. (right) DAC setup for heating under pressure



Diffraction measurements (left) probe how the materials structure changes as it is compressed. $Sc_2(WO_4)_3$ undergoes two phase transitions on compression, the last of which is irreversible on decompression

As part of our work examining the solid state chemistry of negative thermal expansion frameworks we have recently started to examine pressure induced amorphization in negative thermal expansion materials. These experiments have involved current and former Georgia Tech students/postdocs (Cora Lind, Tamas Varga, Mehemet Cetinkol and Andrew Jupe) and collaborators at both the CHiPR (Center for High Pressure Research – an NSF supported center) and Cornell /CHESS (Prof. Bill Basset and Dr. Zha). We are investigating the structural changes that occur in NTE materials as they are compressed and transform to glasses. This amorphization is an important problem in the fabrication of some controlled thermal expansion composite materials. Several different mechanisms have been proposed for the amorphization by other workers and it has even been proposed that the amorphization is intimately tied to the NTE characteristics of the starting material. We are examining both the structure of glasses recovered from high pressure, using X-ray absorption spectroscopy, and the structure of materials as they are amorphized in a diamond anvil cell using a combination of *in-situ* X-ray absorption spectroscopy and diffraction. The structural studies are being performed at CHESS, an NSF supported synchrotron facility located on the campus of Cornell University. The structural information that we are obtaining will help us distinguish between different possible amorphization mechanisms.

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Education:

Five graduate students (Cora Lind, Tamas Varga, Kathy White and Mehmet Cetinkol, Mehmet Kutukcu), an undergraduate (Michael Morant) and a postdoc (Andrew Jupe) have contributed to our work on NTE materials. Cora, after spending a postdoctoral period at Cornell, has recently joined the chemistry faculty at the University of Toledo, OH.

Cora adjusts a cryostat prior to an experiment at the Advanced Photon Source

Outreach:

The PI is involved in running a (separately NSF supported) summer program for chemistry undergraduates and faculty from schools with little or no research activity.

The 2004 group of summer students relaxing after a hard day during the tutorial week at Clemson